

# Semi-Supervised learning with Density-Ratio Estimation

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## Abstract

In this paper, we study statistical properties of semi-supervised learning, which is considered as an important problem in the community of machine learning. In the standard supervised learning, only the labeled data is observed. The classification and regression problems are formalized as the supervised learning. In semi-supervised learning, unlabeled data is also obtained in addition to labeled data. Hence, exploiting unlabeled data is important to improve the prediction accuracy in semi-supervised learning. This problem is regarded as a semiparametric estimation problem with missing data. Under the discriminative probabilistic models, it had been considered that the unlabeled data is useless to improve the estimation accuracy. Recently, it was revealed that the weighted estimator using the unlabeled data achieves better prediction accuracy in comparison to the learning method using only labeled data, especially when the discriminative probabilistic model is misspecified. That is, the improvement under the semiparametric model with missing data is possible, when the semiparametric model is misspecified. In this paper, we apply the density-ratio estimator to obtain the weight function in the semi-supervised learning. The benefit of our approach is that the proposed estimator does not require well-specified probabilistic models for the probability of the unlabeled data. Based on the statistical asymptotic theory, we prove that the estimation accuracy of our method outperforms the supervised learning using only labeled data. Some numerical experiments present the usefulness of our methods.

## 1 Introduction

In this paper, we analyze statistical properties of semi-supervised learning. In the standard supervised learning, only the labeled data  $(x, y)$  is observed, and the goal is to estimate the relation between  $x$  and  $y$ . In semi-supervised learning (Chapelle et al., 2006), the unlabeled data  $x'$  is also obtained in addition to labeled data. In real-world data such as the text data, we can often obtain both labeled and unlabeled data. A typical example is that  $x$  and  $y$  stand for the text of an article, and the tag of the article, respectively. Tagging the article demands a lot of effort. Hence, the labeled data is scarce, while the unlabeled data is abundant. In semi-supervised learning, studying methods of exploiting unlabeled data is an important issue.

In the standard semi-supervised learning, statistical models of the joint probability  $p(x, y)$ , i.e., generative models, are often used to incorporate the information involved in the unlabeled data into the estimation. For example, under the statistical model  $p(x, y; \beta)$  having the parameter  $\beta$ , the information involved in the unlabeled data is used to estimate the parameter  $\beta$  via the marginal probability  $p(x; \beta) = \int p(x, y; \beta) dy$ . The amount of information in unlabeled samples is studied by (Castelli & Cover, 1996; Dillon et al., 2010; Sinha & Belkin, 2007). This approach is developed to deal with a various data structures. For example, semi-supervised

learning with manifold assumption or cluster assumption has been studied along this line (Belkin & Niyogi, 2004; Lafferty & Wasserman, 2007). Under some assumptions on generative models, it is revealed that unlabeled data is useful to improve the prediction accuracy.

Statistical models of the conditional probability  $p(y|x)$ , i.e., discriminative models, are also used in semi-supervised learning. It seems that the unlabeled data is not useful that much for the estimation of the conditional probability, since the marginal probability does not have any information on  $p(y|x)$  (Lasserre et al., 2006; Seeger, 2001; Zhang & Oles, 2000). Indeed, the maximum likelihood estimator using a parametric model of  $p(y|x)$  is not affected by the unlabeled data. Sokolovska, et al. (Sokolovska et al., 2008), however, proved that even under discriminative models, unlabeled data is still useful to improve the prediction accuracy of the learning method with only labeled data.

Semi-supervised learning methods basically work well under some assumptions on the population distribution and the statistical models. However, it was also reported that the semi-supervised learning has a possibility to degrade the estimation accuracy, especially when a misspecified model is applied (Cozman et al., 2003; Grandvalet & Bengio, 2005; Nigam et al., 1999). Hence, a *safe* semi-supervised learning is desired. The learning algorithms proposed by Sokolovska, et al. (Sokolovska et al., 2008) and Li and Zhou (Li & Zhou, 2011) have a theoretical guarantee such that the unlabeled data does not degrade the estimation accuracy.

In this paper, we develop the study of (Sokolovska et al., 2008). To incorporate the information involved in unlabeled data into the estimator, Sokolovska, et al. (Sokolovska et al., 2008) used the weighted estimator. In the estimation of the weight function, a well-specified model for the marginal probability  $p(x)$  was assumed. This is a strong assumption for semi-supervised learning. To overcome the drawback, we apply the density-ratio estimator for the estimation of the weight function (Sugiyama & Kawanabe, 2012; Sugiyama et al., 2012). We prove that the semi-supervised learning with the density-ratio estimation improves the standard supervised learning. Our method is available not only classification problems but also regression problems, while many semi-supervised learning methods focus on binary classification problems.

This paper is organized as follows. In Section 2, we show the problem setup. In Section 3, we introduce the weighted estimator investigated by Sokolovska, et al., (Sokolovska et al., 2008). In Section 4, we briefly explain the density-ratio estimation. In Section 5, the asymptotic variance of the estimators under consideration is studied. Section 6 is devoted to prove that the weighted estimator using labeled and unlabeled data outperforms the supervised learning using only labeled data. In Section 7, numerical experiments are presented. We conclude in Section 8.

## 2 Problem Setup

We introduce the problem setup. We suppose that the probability distribution of training samples is given as

$$(x_i, y_i) \sim_{i.i.d.} p(y|x)p(x), \quad i = 1, \dots, n, \quad x'_j \sim_{i.i.d.} q(x), \quad j = 1, \dots, n', \quad (1)$$

where  $p(y|x)$  is the conditional probability of  $y \in \mathcal{Y}$  given  $x \in \mathcal{X}$ , and  $p(x)$  and  $q(x)$  are the marginal probabilities on  $\mathcal{X}$ . Here,  $q(x)$  is regarded as the probability in the testing phase, i.e., the test data  $(x, y)$  is distributed from the joint probability  $p(y|x)q(x)$ , and the estimation accuracy is evaluated under the test probability. The paired sample  $(x_i, y_i)$  is called “labeled

data”, and the unpaired sample  $x'_j$  is called “unlabeled data”. Our goal is to estimate the conditional probability  $p(y|x)$  or the conditional expectation  $E[y|x]$  based on the labeled and unlabeled data in (1). When  $\mathcal{Y}$  is a finite set, the problem is called the classification problem. For  $\mathcal{Y} = \mathbb{R}$ , the estimation of  $E[y|x]$  is referred to as the regression problem.

We describe the assumption on the marginal distributions,  $p(x)$  and  $q(x)$  in (1). In the context of the *covariate shift* adaptation (Shimodaira, 2000), the assumption that  $p(x) \neq q(x)$  is employed in general. The weighted estimator with the weight function  $q(x)/p(x)$  is used to correct the estimation bias induced by the covariate shift; see (Sugiyama & Kawanabe, 2012; Sugiyama et al., 2012) for details. Hence, the estimation of the weight function  $q(x)/p(x)$  is important to achieve a good estimation accuracy. On the other hand, in the *semi-supervised learning* (Chapelle et al., 2006), the equality  $p(x) = q(x)$  is assumed, and often  $n'$  is much larger than  $n$ . This setup is also quite practical. For example, in the text data mining, the labeled data is scarce, while the unlabeled data is abundant. In this paper, we assume that the equality

$$p(x) = q(x) \quad (2)$$

holds.

We define the following semiparametric model,

$$\mathcal{M} = \left\{ p(y|x; \boldsymbol{\alpha})r(x) : \boldsymbol{\alpha} \in A \subset \mathbb{R}^d, r \in \mathcal{P} \right\}, \quad (3)$$

for the estimation of the conditional probability  $p(y|x)$ , where  $\mathcal{P}$  is the set of all probability densities of the covariate  $x$ . The parameter of interest is  $\boldsymbol{\alpha}$ , and  $r(x) \in \mathcal{P}$  is the nuisance parameter. The model  $\mathcal{M}$  does not necessarily include the true probability  $p(y|x)q(x)$ , i.e., there may not exist the parameter  $\boldsymbol{\alpha}$  such that  $p(y|x) = p(y|x; \boldsymbol{\alpha})$  holds. This is the significant condition, when we consider the improvement of the inference with the labeled and unlabeled data. Our target is to estimate the parameter  $\boldsymbol{\alpha}^*$  satisfying

$$\max_{\boldsymbol{\alpha} \in A} E[\log p(y|x; \boldsymbol{\alpha})] = E[\log p(y|x; \boldsymbol{\alpha}^*)], \quad (4)$$

in which  $E[\cdot]$  denotes the expectation with respect to the population distribution. If the model  $\mathcal{M}$  includes the true probability, we have  $p(y|x; \boldsymbol{\alpha}^*) = p(y|x)$  due to the non-negativity of Kullback-Leibler divergence (Cover & Thomas, 2006). In the misspecified setup, however, the equality  $p(y|x; \boldsymbol{\alpha}^*) = p(y|x)$  is not guaranteed.

### 3 Weighted Estimator in Semi-supervised Learning

We introduce the weighted estimator. For the estimation of  $p(y|x)$  under the model (3), we consider the maximum likelihood estimator (MLE). For the statistical model  $p(y|x; \boldsymbol{\alpha})$ , let  $\mathbf{u}(x, y; \boldsymbol{\alpha}) \in \mathbb{R}^d$  be the score function

$$\mathbf{u}(x, y; \boldsymbol{\alpha}) = \nabla \log p(y|x; \boldsymbol{\alpha}),$$

where  $\nabla$  denotes the gradient with respect to the model parameter. Then, for any  $\boldsymbol{\alpha} \in A$ , we have

$$\int \mathbf{u}(x, y; \boldsymbol{\alpha}) p(y|x; \boldsymbol{\alpha}) p(x) dx dy = \mathbf{0}.$$

In addition, the extremal condition of (4) leads to

$$\int \mathbf{u}(x, y; \boldsymbol{\alpha}^*) p(y|x) p(x) dx dy = \mathbf{0}.$$

Hence, we can estimate the conditional density  $p(y|x)$  by  $p(y|x; \hat{\boldsymbol{\alpha}})$ , where  $\hat{\boldsymbol{\alpha}}$  is a solution of the estimation equation

$$\frac{1}{n} \sum_{i=1}^n \mathbf{u}(x_i, y_i; \boldsymbol{\alpha}) = \mathbf{0}. \quad (5)$$

Under the regularity condition, the MLE has the statistical consistency to the parameter  $\boldsymbol{\alpha}^*$  in (4); see (van der Vaart, 1998) for details. In addition, the score function  $\mathbf{u}$  is an optimal choice among Z-estimators (van der Vaart, 1998), when the true probability density is included in the model  $\mathcal{M}$ . This implies that the efficient score of the semiparametric model  $\mathcal{M}$  is the same as the score function of the model  $p(y|x; \boldsymbol{\alpha})$ . This is because, in the semiparametric model  $\mathcal{M}$ , the tangent space of the parameter of interest is orthogonal to that of the nuisance parameter. Here, the asymptotic variance matrix of the estimated parameter is employed to compare the estimation accuracy.

Next, we consider the setup of the semi-supervised learning. When the model  $\mathcal{M}$  is specified, we find that the estimator (5) using only the labeled data is efficient. This is obtained from the results of numerous studies about the semiparametric inference with missing data; see (Nan et al., 2009; Robins et al., 1994) and references therein.

Suppose that the model  $\mathcal{M}$  is misspecified. Then, it is possible to improve the MLE in (5) by using the weighted MLE (Sokolovska et al., 2008). The weighted MLE is defined as a solution of the equation,

$$\frac{1}{n} \sum_{i=1}^n w(x_i) \mathbf{u}(x_i, y_i; \boldsymbol{\alpha}) = \mathbf{0}, \quad (6)$$

where  $w(x)$  is a weight function. Suppose that  $w(x) = q(x)/p(x)$ . Then the law of large numbers leads to the probabilistic convergence,

$$\frac{1}{n} \sum_{i=1}^n w(x_i) \mathbf{u}(x_i, y_i; \boldsymbol{\alpha}) \xrightarrow{p} \int \frac{q(x)}{p(x)} \mathbf{u}(x, y; \boldsymbol{\alpha}) p(y|x) p(x) dx = \int \mathbf{u}(x, y; \boldsymbol{\alpha}) p(y|x) q(x) dx.$$

Hence the estimator  $p(y|x; \hat{\boldsymbol{\alpha}})$  based on (6) will provide a good estimator of  $p(y|x)$  under the marginal probability  $q(x)$ . This indicates that  $p(y|x; \hat{\boldsymbol{\alpha}})$  is expected to approximate  $p(y|x)$  over the region on which  $q(x)$  is large. The weight function  $w(x)$  has a role to adjust the bias of the estimator under the covariate shift (Shimodaira, 2000). On the setup of the semi-supervised learning, however,  $w(x) = q(x)/p(x) = 1$  holds, and it is known beforehand. Hence, one may think that there is no need to estimate the weight function. Sokolovska, et al., (Sokolovska et al., 2008) showed that estimation of the weight function is useful, even though it is already known in the semi-supervised learning.

We briefly introduce the result in (Sokolovska et al., 2008). Let the set  $\mathcal{X}$  be finite. Then,  $\mathcal{P}$  is a finite dimensional parametric model. Suppose that the sample size of the unlabeled data is enormous, and that the probability function  $q(x)$  on  $\mathcal{X}$  is known with a high degree of

accuracy. The probability  $p(x)$  is estimated by the maximum likelihood estimator  $\hat{p}(x)$  based on the samples  $\{x_i\}_{i=1}^n$  in the labeled data. Then, Sokolovska, et al. (Sokolovska et al., 2008) showed that the weighted MLE (6) with the estimated weight function  $w(x) = q(x)/\hat{p}(x)$  improves the naive MLE, when the model  $\mathcal{M}$  is misspecified, i.e.,  $p(y|x)q(x) \notin \mathcal{M}$ .

Shimodaira (Shimodaira, 2000) pointed out that the weighted MLE using the exact density ratio  $w(x) = q(x)/p(x)$  has the statistical consistency to the target parameter  $\alpha^*$ , when the covariate shift occurs. Under the regularity condition, it is rather straightforward to see that the weighted MLE using the estimated weight function  $w(x) = q(x)/\hat{p}(x)$  also converges to  $\alpha^*$  in probability, since  $\hat{p}(x)$  converges to  $p(x)$  in probability. Sokolovska’s result implies that when  $p(x) = q(x)$  holds, the weighted MLE using the estimated weight function improves the weighted MLE using the true density ratio in the sense of the asymptotic variance of the estimator.

The phenomenon above is similar to the statistical paradox analyzed by (Henmi & Eguchi, 2004; Henmi et al., 2007). In the semi-parametric estimation, Henmi and Eguchi (Henmi & Eguchi, 2004) pointed out that the estimation accuracy of the parameter of interest can be improved by estimating the nuisance parameter, even when the nuisance parameter is known beforehand. Hirano, et al., (Hirano et al., 2003) also pointed out that the estimator with the estimated propensity score is more efficient than the estimator using the true propensity score in the estimation of the average treatment effects. Here, the propensity score corresponds to the weight function  $w(x)$  in our context. The degree of improvement is described by using the projection of the score function onto the subspace defined by the efficient score for the semi-parametric model. In our analysis, also the projection of the score function  $u(x, y; \alpha)$  plays an important role as shown in Section 6.

For the estimation of the weight function in (6), we apply the density-ratio estimator (Sugiyama & Kawanabe, 2012; Sugiyama et al., 2012) instead of estimating the probability densities separately. We show that the density-ratio estimator provides a practical method for the semi-supervised learning. In the next section, we introduce the density-ratio estimation.

## 4 Density-ratio estimation

Density-ratio estimators are available to estimate the weight function  $w(x) = q(x)/p(x)$ . Recently, methods of the direct estimation for density-ratios have been developed in the machine learning community (Sugiyama & Kawanabe, 2012; Sugiyama et al., 2012). We apply the density-ratio estimator to estimate the weight function  $w(x)$  instead of using the estimator of each probability density.

We briefly introduce the density-ratio estimator according to (Qin, 1998). Suppose that the following training samples are observed,

$$x_i \sim_{i.i.d.} p(x), \quad i = 1, \dots, n, \quad x'_j \sim_{i.i.d.} q(x), \quad j = 1, \dots, n'. \quad (7)$$

Our goal is to estimate the density-ratio  $w(x) = q(x)/p(x)$ . The  $r$ -dimensional parametric model for the density-ratio is defined by

$$w(x; \theta) = \exp\{\theta_1 \phi_1(x) + \dots + \theta_r \phi_r(x)\}, \quad (8)$$

where  $\phi_1(x) = 1$  is assumed. For any function  $\eta(x; \theta) \in \mathbb{R}^r$  which may depend on the parameter  $\theta$ , one has the equality

$$\int \eta(x; \theta) w(x) p(x) dx - \int \eta(x; \theta) q(x) dx = \mathbf{0}$$

Hence, the empirical approximation of the above equation is expected to provide an estimation equation of the density-ratio. The empirical approximation of the above equality under the parametric model of  $w(x; \boldsymbol{\theta})$  is given as

$$\frac{1}{n} \sum_{i=1}^n \boldsymbol{\eta}(x_i; \boldsymbol{\theta}) w(x_i; \boldsymbol{\theta}) - \frac{1}{n'} \sum_{j=1}^{n'} \boldsymbol{\eta}(x'_j; \boldsymbol{\theta}) = \mathbf{0}. \quad (9)$$

Let  $\hat{\boldsymbol{\theta}}$  be a solution of (9), and then,  $w(x; \hat{\boldsymbol{\theta}})$  is an estimator of  $w(x)$ . Note that we do not need to estimate probability densities  $p(x)$  and  $q(x)$  separately. The estimation equation (9) provides a direct estimator of the density-ratio based on the moment matching with the function  $\boldsymbol{\eta}(x; \boldsymbol{\theta})$ .

Qin (Qin, 1998) proved that the optimal choice of  $\boldsymbol{\eta}(x; \boldsymbol{\theta})$  is given as

$$\boldsymbol{\eta}(x; \boldsymbol{\theta}) = \frac{1}{1 + n'/n \cdot w(x; \boldsymbol{\theta})} \nabla \log w(x; \boldsymbol{\theta}) = \frac{1}{1 + n'/n \cdot w(x; \boldsymbol{\theta})} \boldsymbol{\phi}(x), \quad (10)$$

where  $\boldsymbol{\phi}(x) = (\phi_1(x), \dots, \phi_r(x))^T$ . By using  $\boldsymbol{\eta}(x; \boldsymbol{\theta})$  above, the asymptotic variance matrix of  $\hat{\boldsymbol{\theta}}$  is minimized among the set of moment matching estimators, when  $w(x)$  is realized by the model  $w(x; \boldsymbol{\theta})$ . Hence, (10) is regarded as the counterpart of the score function for parametric probability models.

## 5 Semi-Supervised Learning with Density-Ratio Estimation

We study the asymptotics of the weighted MLE (6) using the estimated density-ratio. The estimation equation is given as

$$\begin{cases} \frac{1}{n} \sum_{i=1}^n w(x_i; \boldsymbol{\theta}) \mathbf{u}(x_i, y_i; \boldsymbol{\alpha}) = \mathbf{0}, \\ \frac{1}{n} \sum_{i=1}^n \boldsymbol{\eta}(x_i; \boldsymbol{\theta}) w(x_i; \boldsymbol{\theta}) - \frac{1}{n'} \sum_{j=1}^{n'} \boldsymbol{\eta}(x'_j; \boldsymbol{\theta}) = \mathbf{0}. \end{cases} \quad (11)$$

Here, the statistical models (3) and (8) are employed. The first equation is used for the estimation of the parameter  $\boldsymbol{\alpha}$  of the model  $p(y|x; \boldsymbol{\alpha})$ , and the second equation is used for the estimation of the density-ratio  $w(x; \boldsymbol{\theta})$ . The estimator defined by (11) is referred to as density-ratio estimation based on semi supervised learning, or *DRESS* for short.

In Sokolovska, et al. (Sokolovska et al., 2008), the marginal probability density  $p(x)$  is estimated by using a well-specified parametric model. Clearly, preparing the well-specified parametric model is not practical, when  $\mathcal{X}$  is not finite set. On the other hand, it is easy to prepare a specified model of the density-ratio  $w(x)$ , whenever  $p(x) = q(x)$  holds in (1). The model (8) is an example. Indeed,  $w(x; \mathbf{0}) = 1$  holds. Hence, the assumption that the true weight function is realized by the model  $w(x; \boldsymbol{\theta})$  is not of an obstacle in semi-supervised learning.

We show the asymptotic expansion of the estimation equation (11). Let  $\hat{\boldsymbol{\alpha}}$  and  $\hat{\boldsymbol{\theta}}$  be a solution of (11). In addition, define  $\boldsymbol{\alpha}^*$  be a solution of

$$\int \mathbf{u}(x, y; \boldsymbol{\alpha}) p(y|x) p(x) dx dy = \mathbf{0}$$

and  $\boldsymbol{\theta}^*$  be the parameter such that  $w(x; \boldsymbol{\theta}^*) = 1$ , i.e.,  $\boldsymbol{\theta}^* = \mathbf{0}$ . We prepare some notations:  $\mathbf{u} = \mathbf{u}(x, y; \boldsymbol{\alpha}^*)$ ,  $\boldsymbol{\eta} = \boldsymbol{\eta}(x; \boldsymbol{\theta}^*)$ ,  $\mathbf{u}_i = \mathbf{u}(x_i, y_i; \boldsymbol{\alpha}^*)$ ,  $\boldsymbol{\eta}_i = \boldsymbol{\eta}(x_i; \boldsymbol{\theta}^*)$ ,  $\boldsymbol{\eta}'_j = \boldsymbol{\eta}(x'_j; \boldsymbol{\theta}^*)$ ,  $\delta\boldsymbol{\alpha} = \hat{\boldsymbol{\alpha}} - \boldsymbol{\alpha}^*$ ,  $\delta\boldsymbol{\theta} = \hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*$ . The Jacobian of the score function  $\mathbf{u}$  with respect to the parameter  $\boldsymbol{\alpha}$  is denoted as  $\nabla\mathbf{u}$ , i.e., the  $d$  by  $d$  matrix whose element is given as  $(\nabla\mathbf{u}(x, y; \boldsymbol{\alpha}))_{ik} = \frac{\partial^2}{\partial\alpha_i\partial\alpha_k} \log p(y|x; \boldsymbol{\alpha})$ . The variance matrix and the covariance matrix under the probability  $p(y|x)p(x)$  are denoted as  $V[\cdot]$  and  $\text{Cov}[\cdot, \cdot]$ , respectively. Without loss of generality, we assume that  $\boldsymbol{\eta}$  at  $\boldsymbol{\theta} = \boldsymbol{\theta}^*$  is represented as

$$\boldsymbol{\eta}(x; \boldsymbol{\theta}^*) = \boldsymbol{\phi}(x) + \tilde{\boldsymbol{\phi}}(x),$$

where  $\tilde{\boldsymbol{\phi}}(x)$  is an arbitrary function orthogonal to  $\boldsymbol{\phi}(x)$ , i.e.,  $E[\boldsymbol{\phi}\tilde{\boldsymbol{\phi}}^T] = \mathbf{O}$  holds. If  $\boldsymbol{\eta}(x; \boldsymbol{\theta}^*)$  does not have any component which is represented as a linear transformation of  $\boldsymbol{\phi}(x)$ , the estimator would be degenerated. Under the regularity condition, the estimated parameters,  $\hat{\boldsymbol{\alpha}}$  and  $\hat{\boldsymbol{\theta}}$ , converge to  $\boldsymbol{\alpha}^*$  and  $\boldsymbol{\theta}^*$ , respectively. The asymptotic expansion of (11) around  $(\boldsymbol{\alpha}, \boldsymbol{\theta}) = (\boldsymbol{\alpha}^*, \boldsymbol{\theta}^*)$  leads to

$$\begin{aligned} E[\nabla\mathbf{u}]\delta\boldsymbol{\alpha} + E[\mathbf{u}\boldsymbol{\phi}^T]\delta\boldsymbol{\theta} &= -\frac{1}{n} \sum_{i=1}^n \mathbf{u}_i + o_p(n^{-1/2}), \\ E[\boldsymbol{\phi}\boldsymbol{\phi}^T]\delta\boldsymbol{\theta} &= \frac{1}{n'} \sum_{j=1}^{n'} \boldsymbol{\eta}'_j - \frac{1}{n} \sum_{i=1}^n \boldsymbol{\eta}_i + o_p(n^{-1/2}). \end{aligned}$$

Hence, we have

$$E[\nabla\mathbf{u}]\delta\boldsymbol{\alpha} = \frac{1}{n} \sum_{i=1}^n \{E[\mathbf{u}\boldsymbol{\phi}^T]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}\boldsymbol{\eta}_i - \mathbf{u}_i\} - \frac{1}{n'} \sum_{j=1}^{n'} E[\mathbf{u}\boldsymbol{\phi}^T]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}\boldsymbol{\eta}'_j + o_p(n^{-1/2}).$$

Therefore, we obtain the asymptotic variance,

$$\begin{aligned} & n \cdot E[\nabla\mathbf{u}]V[\delta\boldsymbol{\alpha}]E[\nabla\mathbf{u}]^T \\ &= V[\mathbf{u}] + \left(1 + \frac{n}{n'}\right) E[\mathbf{u}\boldsymbol{\phi}^T]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}V[\boldsymbol{\eta}]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}E[\boldsymbol{\phi}\mathbf{u}^T] \\ &\quad - E[\mathbf{u}\boldsymbol{\phi}^T]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}\text{Cov}[\boldsymbol{\eta}, \mathbf{u}] - \text{Cov}[\mathbf{u}, \boldsymbol{\eta}]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}E[\boldsymbol{\phi}\mathbf{u}^T] + o(1) \end{aligned}$$

On the other hand, the variance of the naive MLE,  $\tilde{\boldsymbol{\alpha}}$ , defined as a solution of (5) is given as

$$n \cdot E[\nabla\mathbf{u}]V[\delta\tilde{\boldsymbol{\alpha}}]E[\nabla\mathbf{u}]^T = V[\mathbf{u}] + o(1),$$

where  $\delta\tilde{\boldsymbol{\alpha}} = \tilde{\boldsymbol{\alpha}} - \boldsymbol{\alpha}^*$ .

## 6 Maximum Improvement by Semi-Supervised Learning

Given the model for the density-ratio  $w(x; \boldsymbol{\theta})$ , we compare the asymptotic variance matrices of the estimators,  $\tilde{\boldsymbol{\alpha}}$  and  $\hat{\boldsymbol{\alpha}}$ . First, let us define

$$\bar{\mathbf{u}}(x) = \int \mathbf{u}(x, y; \boldsymbol{\alpha}^*)p(y|x)dy,$$

i.e.,  $\bar{\mathbf{u}}(x)$  is the projection of the score function  $\mathbf{u}(x, y; \boldsymbol{\alpha}^*)$  onto the subspace consisting of all functions depending only on  $x$ , where the inner product is defined by the expectation under the joint probability  $p(y|x)p(x)$ . Note that the equality  $E[\bar{\mathbf{u}}] = \mathbf{0}$  holds. Let the matrix  $B$  be

$$B = E[\bar{\mathbf{u}}\boldsymbol{\phi}^T]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}.$$

Then, a simple calculation yields that the difference of the variance matrix between  $\tilde{\boldsymbol{\alpha}}$  and  $\hat{\boldsymbol{\alpha}}$  is equal to

$$\begin{aligned} \text{Diff}[\mathbf{u}] &:= n \cdot E[\nabla \mathbf{u}]V[\delta \tilde{\boldsymbol{\alpha}}]E[\nabla \mathbf{u}]^T - n \cdot E[\nabla \mathbf{u}]V[\delta \boldsymbol{\alpha}]E[\nabla \mathbf{u}]^T \\ &= \frac{n'}{n+n'}E[\bar{\mathbf{u}}\bar{\mathbf{u}}^T] - \left(1 + \frac{n}{n'}\right)V[B\boldsymbol{\eta} - \frac{n'}{n+n'}\bar{\mathbf{u}}] + o(1). \end{aligned} \quad (12)$$

In the second equality, we supposed that  $n'/n$  converges to a positive constant. When  $\text{Diff}[\mathbf{u}]$  is positive definite, the estimator  $\hat{\boldsymbol{\alpha}}$  using the labeled and unlabeled data improves the estimator  $\tilde{\boldsymbol{\alpha}}$  using only the labeled data. It is straightforward to see that the improvement is not attained if  $\bar{\mathbf{u}} = \mathbf{0}$  holds. In general, the score function  $\mathbf{u}(x, y; \boldsymbol{\alpha}) = \nabla \log p(y|x; \boldsymbol{\alpha})$  satisfies  $\bar{\mathbf{u}} = \mathbf{0}$ , if the model is specified. When the model of the conditional probability  $p(y|x)$  is misspecified, however, there is a possibility that the proposed estimator (11) outperforms the MLE  $\tilde{\boldsymbol{\alpha}}$ .

We derive the optimal moment function  $\boldsymbol{\eta}$  for the estimation of the parameter  $\boldsymbol{\alpha}^*$ . The optimal  $\boldsymbol{\eta}$  can be different from (10). We prepare some notations. Let  $\Pi_{\boldsymbol{\phi}}\bar{\mathbf{u}}$  be the  $\mathbb{R}^d$ -valued function on  $\mathcal{X}$ , each element of which is the projection of each element of  $\bar{\mathbf{u}}$  onto the subspace spanned by  $\{\phi_1(x), \dots, \phi_r(x)\}$ . Here, the inner product is defined by the expectation under the marginal probability  $p(x)$ . In addition, let  $\Pi_{\boldsymbol{\phi}}^\perp \bar{\mathbf{u}}$  be the projection of  $\bar{\mathbf{u}}$  onto the orthogonal complement of the subspace, i.e.,  $\Pi_{\boldsymbol{\phi}}^\perp \bar{\mathbf{u}} = \bar{\mathbf{u}} - \Pi_{\boldsymbol{\phi}}\bar{\mathbf{u}}$ .

**Theorem 1.** *We assume that the model of the density-ratio is defined as*

$$w(x; \boldsymbol{\theta}) = \exp\{\boldsymbol{\phi}(x)^T \boldsymbol{\theta}\}$$

*with the basis functions  $\boldsymbol{\phi}(x) = (\phi_1(x), \dots, \phi_r(x))$  satisfying  $\phi_1(x) = 1$ . Suppose that  $E[\boldsymbol{\phi}\boldsymbol{\phi}^T] \in \mathbb{R}^{r \times r}$  is invertible, and that the rank of  $E[\bar{\mathbf{u}}\boldsymbol{\phi}^T]E[\boldsymbol{\phi}\boldsymbol{\phi}^T]^{-1}$  is equal to the dimension of the parameter  $\boldsymbol{\alpha}$ , i.e., row full rank. We assume that the moment function  $\boldsymbol{\eta}(x; \boldsymbol{\theta})$  at  $\boldsymbol{\theta} = \boldsymbol{\theta}^*$  is represented as*

$$\boldsymbol{\eta}(x; \boldsymbol{\theta}^*) = \boldsymbol{\phi}(x) + \tilde{\boldsymbol{\phi}}(x) \quad (13)$$

*where  $\tilde{\boldsymbol{\phi}}(x)$  is a function orthogonal to  $\boldsymbol{\phi}(x)$ , i.e.,  $E[\boldsymbol{\phi}(x)\tilde{\boldsymbol{\phi}}(x)^T] = \mathbf{0}$  holds. Then, an optimal  $\tilde{\boldsymbol{\phi}}$  is given as*

$$\tilde{\boldsymbol{\phi}} = \frac{n'}{n+n'}B^T(BB^T)^{-1}\Pi_{\boldsymbol{\phi}}^\perp \bar{\mathbf{u}}. \quad (14)$$

*For the optimal choice of  $\boldsymbol{\eta}$ , the maximum improvement is given as*

$$\begin{aligned} \text{Diff}[\mathbf{u}] &= \frac{n'}{n+n'}E[\bar{\mathbf{u}}\bar{\mathbf{u}}^T] - \frac{n^2}{n'(n+n')}E[\Pi_{\boldsymbol{\phi}}\bar{\mathbf{u}}(\Pi_{\boldsymbol{\phi}}\bar{\mathbf{u}})^T] + o(1) \\ &= \frac{n'}{n+n'}E[\Pi_{\boldsymbol{\phi}}^\perp \bar{\mathbf{u}}(\Pi_{\boldsymbol{\phi}}^\perp \bar{\mathbf{u}})^T] + \frac{n'-n}{n'}E[\Pi_{\boldsymbol{\phi}}\bar{\mathbf{u}}(\Pi_{\boldsymbol{\phi}}\bar{\mathbf{u}})^T] + o(1) \end{aligned} \quad (15)$$



*Proof.* Due to  $\phi_1(x) = 1$ , one has  $E[\tilde{\phi}] = \mathbf{0}$  and  $E[\Pi_{\phi}^{\perp} \bar{\mathbf{u}}] = E[1 \cdot \Pi_{\phi}^{\perp} \bar{\mathbf{u}}] = \mathbf{0}$ . Hence, one has  $E[\Pi_{\phi} \bar{\mathbf{u}}] = E[\bar{\mathbf{u}}] - E[\Pi_{\phi}^{\perp} \bar{\mathbf{u}}] = \mathbf{0}$ . Our goad is to find  $\tilde{\phi}$  which minimizes  $V[B\boldsymbol{\eta} - \frac{n'}{n+n'} \bar{\mathbf{u}}]$  in (12) in the sense of positive definiteness. The orthogonal decomposition leads to

$$V[B\boldsymbol{\eta} - \frac{n'}{n+n'} \bar{\mathbf{u}}] = V[B\phi - \frac{n'}{n+n'} \Pi_{\phi} \bar{\mathbf{u}}] + V[B\tilde{\phi} - \frac{n'}{n+n'} \Pi_{\phi}^{\perp} \bar{\mathbf{u}}],$$

because of the orthogonality between  $B\phi - \frac{n'}{n+n'} \Pi_{\phi} \bar{\mathbf{u}}$  and  $B\tilde{\phi} - \frac{n'}{n+n'} \Pi_{\phi}^{\perp} \bar{\mathbf{u}}$ , and the equality  $E[B\tilde{\phi} - \frac{n'}{n+n'} \Pi_{\phi}^{\perp} \bar{\mathbf{u}}] = \mathbf{0}$ . Hence,  $\tilde{\phi}$  satisfying

$$B\tilde{\phi} = \frac{n'}{n+n'} \Pi_{\phi}^{\perp} \bar{\mathbf{u}}$$

is an optimal choice. Since the matrix  $B$  is row full rank, a solution of the above equation is given by

$$\tilde{\phi} = \frac{n'}{n+n'} B^T (BB^T)^{-1} \Pi_{\phi}^{\perp} \bar{\mathbf{u}}.$$

We obtain the maximum improvement of  $\text{Diff}[\mathbf{u}]$  by using the equalities  $V[\Pi_{\phi} \bar{\mathbf{u}}] = E[\Pi_{\phi} \bar{\mathbf{u}} (\Pi_{\phi} \bar{\mathbf{u}})^T]$  and  $B\phi = E[\bar{\mathbf{u}} \phi^T] E[\phi \phi^T]^{-1} \phi = \Pi_{\phi} \bar{\mathbf{u}}$ .  $\square$

Suppose that the optimal moment function  $\boldsymbol{\eta} = \phi + \tilde{\phi}$  presented in Theorem 1 is used with the score function  $\mathbf{u}(x, y; \boldsymbol{\alpha})$ . Then, the improvement (15) is maximized when  $E[\Pi_{\phi} \bar{\mathbf{u}} (\Pi_{\phi} \bar{\mathbf{u}})^T]$  is minimized. Hence, the model  $w(x; \boldsymbol{\theta})$  with the lower dimensional parameter  $\boldsymbol{\theta}$  is preferable as long as the assumption in Theorem 1 is satisfied. This is intuitively understandable, because the statistical perturbation of the density-ratio estimator is minimized, when the smallest model is employed.

**Remark 1.** Suppose that the basis functions,  $\phi_1(x), \dots, \phi_r(x)$ , are closely orthogonal to  $\bar{\mathbf{u}}$ , i.e.,  $E[\bar{\mathbf{u}} \phi^T]$  is close to the null matrix. Then, the improvement  $\text{Diff}[\mathbf{u}]$  is close to  $\frac{n'}{n+n'} E[\bar{\mathbf{u}} \bar{\mathbf{u}}^T]$ . As a result, we have  $\sup_{\phi} \text{Diff}[\mathbf{u}] = \frac{n'}{n+n'} E[\bar{\mathbf{u}} \bar{\mathbf{u}}^T]$  in which the supremum is taken over the basis of the density-ratio model satisfying the assumption in Theorem 1. However, the basis functions satisfying the exact equality  $E[\bar{\mathbf{u}} \phi^T] = O$  is useless. Because, the equality  $E[\bar{\mathbf{u}} \phi^T] = O$  leads to  $B = O$  and thus, the equality (12) is reduced to

$$\text{Diff}[\mathbf{u}] = \frac{n'}{n+n'} E[\bar{\mathbf{u}} \bar{\mathbf{u}}^T] - \frac{n+n'}{n'} V[\frac{n'}{n+n'} \bar{\mathbf{u}}] + o(1) = o(1).$$

This result implies that there is the singularity at the basis function  $\phi$  such that  $E[\bar{\mathbf{u}} \phi^T] = O$ .

It is not practical to apply the optimal function  $\boldsymbol{\eta}(x; \boldsymbol{\theta})$  defined by (14). The optimal moment function depends on  $\bar{\mathbf{u}}$ , and one needs information on the probability  $p(y|x)$  to obtain the explicit form of  $\bar{\mathbf{u}}$ . The estimation of  $\bar{\mathbf{u}}$  needs non-parametric estimation, since the model misspecification of  $\mathcal{M}$  is significant in our setup. Thus, we consider more practical estimator for the density ratio. Suppose that  $\tilde{\phi} = \mathbf{0}$  holds for the moment function  $\boldsymbol{\eta}(x; \boldsymbol{\theta}^*)$ . For example, the optimal moment function (10) satisfies  $\boldsymbol{\eta}(x; \boldsymbol{\theta}^*) = \frac{n}{n+n'} \phi(x)$  at  $\boldsymbol{\theta} = \boldsymbol{\theta}^*$ , i.e.,  $\tilde{\phi} = \mathbf{0}$ . For the

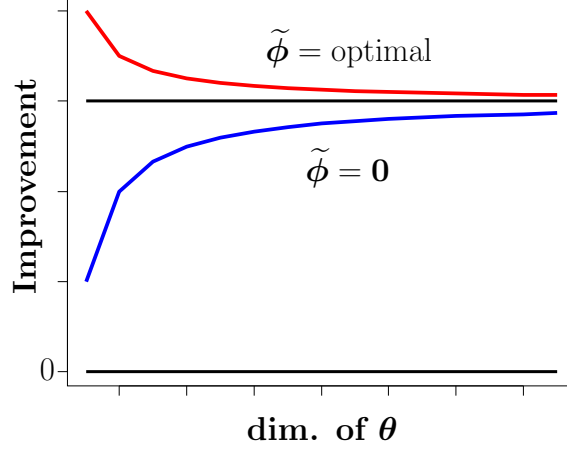


Figure 1: The improvement  $\text{Diff}[\mathbf{u}]$  is depicted as the function of the dimension of the density-ratio model. Since the improvement is represented by the matrix, the figure gives a view showing a frame format of the inequality relation. When the dimension of  $\boldsymbol{\theta}$  tends to infinity and  $n' > n$  holds, the two curves converges to the common positive definite matrix  $\frac{n'-n}{n'}E[\bar{\mathbf{u}}\bar{\mathbf{u}}^T]$ .

density-ratio model  $w(x; \boldsymbol{\theta}) = \exp\{\boldsymbol{\phi}(x)^T \boldsymbol{\theta}\}$  with  $\phi_1(x) = 1$  and the moment function satisfying  $\boldsymbol{\eta}(x; \boldsymbol{\theta}^*) = \boldsymbol{\phi}(x)$ , a brief calculation yields that

$$\text{Diff}[\mathbf{u}] = \frac{n' - n}{n'} E[\Pi_{\boldsymbol{\phi}} \bar{\mathbf{u}} (\Pi_{\boldsymbol{\phi}} \bar{\mathbf{u}})^T] + o(1). \quad (16)$$

Hence, the improvement is attained, when  $n < n'$  holds. As an interesting fact, we see that the larger model  $w(x; \boldsymbol{\theta})$  attains the better improvement in (16). Indeed,  $\Pi_{\boldsymbol{\phi}} \bar{\mathbf{u}}$  gets close to  $\bar{\mathbf{u}}$ , when the density-ratio model  $w(x; \boldsymbol{\theta}) = \exp\{\boldsymbol{\theta}^T \boldsymbol{\phi}(x)\}$  becomes large. Hence, the non-parametric estimation of the density-ratio may be a good choice to achieve a large improvement for the estimation of the conditional probability. This is totally different from the case that the optimal  $\tilde{\boldsymbol{\phi}}$  presented in Theorem 1 is used in the density-ratio estimation. The relation between  $\text{Diff}[\mathbf{u}]$  using the optimal  $\tilde{\boldsymbol{\phi}}$  and  $\text{Diff}[\mathbf{u}]$  with  $\tilde{\boldsymbol{\phi}} = \mathbf{0}$  is illustrated in Figure 1. In the limit of the dimension of  $\boldsymbol{\theta}$ , both variance matrices converge to  $\frac{n'-n}{n'}E[\bar{\mathbf{u}}\bar{\mathbf{u}}^T]$  monotonically.

**Example 1.** Let  $\mathbf{u}(x, y; \boldsymbol{\alpha})$  be the score function of the model  $y = \boldsymbol{\alpha}^T \mathbf{b}(x) + Z$ ,  $Z \sim N(0, \sigma^2)$ , where  $\mathbf{b}(x) = (b_1(x), \dots, b_d(x))$  is the vector consisting of basis functions and  $\sigma^2$  is a known parameter. Then, one has  $\mathbf{u}(x, y; \boldsymbol{\alpha}) = (y - \boldsymbol{\alpha}^T \mathbf{b}(x)) \mathbf{b}(x)$ . Suppose that the true conditional probability leads to the regression function  $y = f(x) + Z$ , where  $E[Z|x] = 0$  for all  $x$ . Then, one has  $\bar{\mathbf{u}}(x; \boldsymbol{\alpha}) = (f(x) - \boldsymbol{\alpha}^T \mathbf{b}(x)) \mathbf{b}(x)$  and  $E[\bar{\mathbf{u}}\bar{\mathbf{u}}^T] = E[(f(x) - \boldsymbol{\alpha}^T \mathbf{b}(x))^2 \mathbf{b}(x) \mathbf{b}(x)^T]$ . Hence, the upper bound of the improvement is governed by the degree of the model misspecification  $(f(x) - \boldsymbol{\alpha}^T \mathbf{b}(x))^2$ . According to Theorem 1, an optimal moment function  $\boldsymbol{\eta}(x; \boldsymbol{\theta})$  is given as

$$\boldsymbol{\eta}(x; \boldsymbol{\theta}^*) = \boldsymbol{\phi}(x) + \frac{n'}{n + n'} B^T (B B^T)^{-1} ((f(x) - \boldsymbol{\alpha}^{*T} \mathbf{b}(x)) \mathbf{b}(x) - B \boldsymbol{\phi}(x))$$

at  $\boldsymbol{\theta} = \boldsymbol{\theta}^*$ , where  $B = E[(f - \boldsymbol{\alpha}^{*T} \mathbf{b}) \mathbf{b} \boldsymbol{\phi}^T] E[\boldsymbol{\phi} \boldsymbol{\phi}^T]^{-1}$ .

## 7 Numerical Experiments

We show numerical experiments to compare the standard supervised learning and the semi-supervised learning using DRESS. Both regression problems and classification problems are presented.

### 7.1 Regression problems

We consider the regression problem with the  $d$ -dimensional covariate variable shown below.

**labeled data:**

$$\begin{aligned} y_i &= \mathbf{1}^T \mathbf{x}_i + \varepsilon \frac{\|\mathbf{x}_i\|^2}{d} + z_i, \quad z_i \sim N(0, \sigma^2), \quad i = 1, \dots, n, \\ \mathbf{x}_i &\sim N_d(\mathbf{0}, I_d), \quad \mathbf{1}^T = (1, \dots, 1) \in \mathbb{R}^d. \end{aligned} \quad (17)$$

**unlabeled data:**  $\mathbf{x}'_j \sim N_d(\mathbf{0}, I_d)$ ,  $j = 1, \dots, n'$ .

**regression model:**  $y = \boldsymbol{\alpha}^T \mathbf{x} + z$ ,  $\boldsymbol{\alpha} \in \mathbb{R}^d$ ,  $z \sim N(0, s^2)$ .

**score function:**  $u(x, y; \boldsymbol{\alpha}) = (y - \boldsymbol{\alpha}^T \mathbf{x})\mathbf{x}$ .

The parameter  $\varepsilon$  in (17) implies the degree of the model misspecification. Let  $f_\varepsilon$  be the target function,  $f_\varepsilon(\mathbf{x}) = \mathbf{1}^T \mathbf{x} + \varepsilon \|\mathbf{x}\|^2/d$ , and define

$$e(\varepsilon) = \min_{\boldsymbol{\alpha}} E_{\mathbf{x}}[|f_\varepsilon(\mathbf{x}) - \boldsymbol{\alpha}^T \mathbf{x}|^2],$$

which implies the squared distance from the true function  $f_\varepsilon$  to the linear regression model. On the other hand, the mean square error of the naive least mean square (LMS) estimator  $\tilde{\boldsymbol{\alpha}}$ , i.e.,  $E_{\text{Data}}[E_{\mathbf{x}}[|f_0(\mathbf{x}) - \tilde{\boldsymbol{\alpha}}^T \mathbf{x}|^2]]$ , is asymptotically equal to  $\sigma^2 d/n$ , when the model is specified. We use the ratio

$$\delta = \sqrt{e(\varepsilon)} / \sqrt{\frac{\sigma^2 d}{n}} = \sqrt{\frac{e(\varepsilon)n}{\sigma^2 d}}$$

as the normalized measure of the model misspecification. When  $\delta \gg 1$  holds, the misspecification of the model can be statistically detected.

First, we use a parametric model for density ratio estimation. For any positive integer  $k$ , let  $\mathbf{x}^{(k)}$  be the  $d$ -dimensional vector  $(x_1^k, \dots, x_d^k)^T$ . The density-ratio model is defined as

$$w(\mathbf{x}; \boldsymbol{\theta}) = \exp \left\{ \theta_0 + \boldsymbol{\theta}_1^T \mathbf{x} + \boldsymbol{\theta}_2^T \mathbf{x}^{(2)} + \dots + \boldsymbol{\theta}_L^T \mathbf{x}^{(L)} \right\}$$

having  $Ld + 1$  dimensional parameter  $(\theta_0, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_L)$ . We apply the estimator (10) presented by Qin (Qin, 1998). Note that the estimator (10) satisfies  $\tilde{\boldsymbol{\phi}} = \mathbf{0}$  at  $\boldsymbol{\theta} = \boldsymbol{\theta}^*$ . Hence, the improvement is asymptotically given by (16). Under the setup of  $d = 2, n = 500, n' = 5000$  and  $\sigma = 0.2$ , we compute the mean square errors for LMS estimator  $\tilde{\boldsymbol{\alpha}}$  and DRESS  $\hat{\boldsymbol{\alpha}}$ . The difference of test errors,

$$n \cdot (E[(\tilde{\boldsymbol{\alpha}}^T \mathbf{x} - f_\varepsilon(\mathbf{x}))^2] - E[(\hat{\boldsymbol{\alpha}}^T \mathbf{x} - f_\varepsilon(\mathbf{x}))^2]),$$

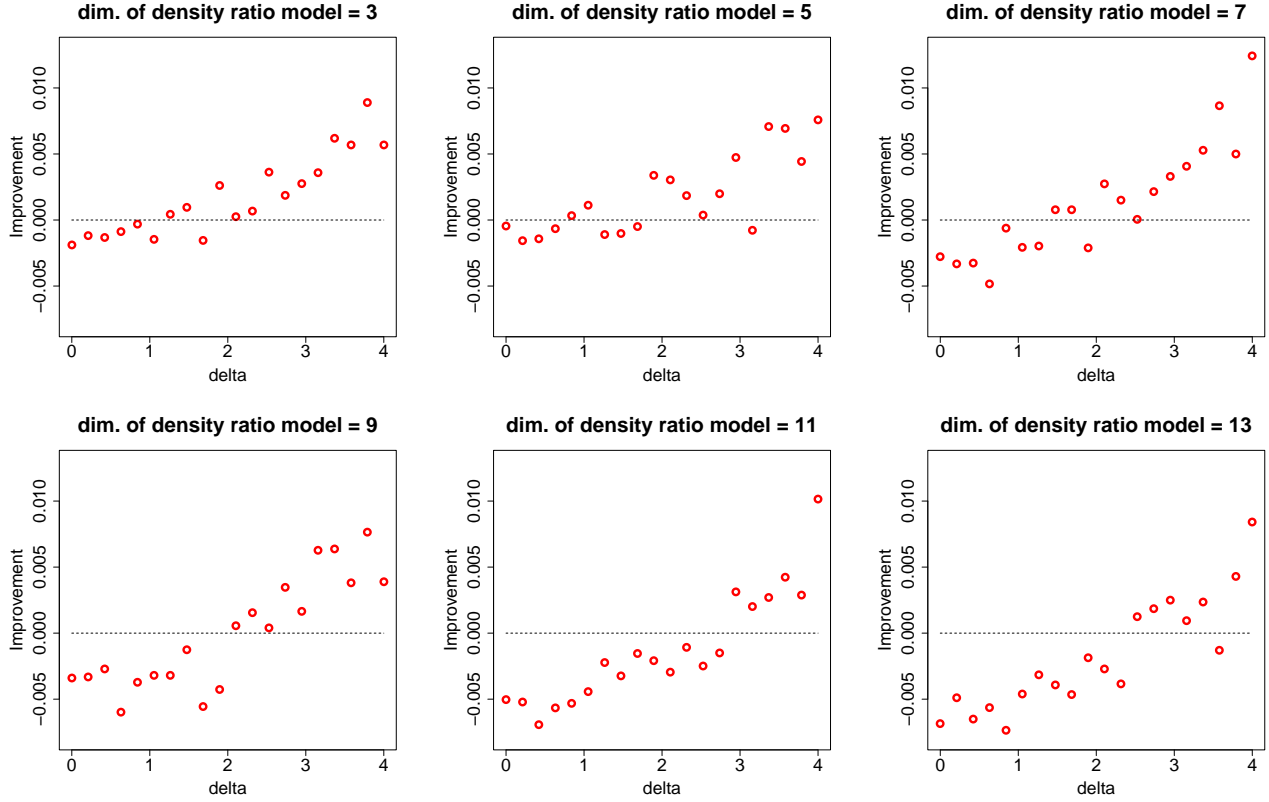


Figure 2: The difference of the mean square errors is plotted as the function of  $\delta$ , where  $\delta$  is the normalized measure of the model misspecification. The vertical axes “Improvement” denotes the difference of the mean square errors between LMS estimator and DRESS. Positive improvement denotes that DRESS outperforms LMS estimator.

is evaluated for each  $\varepsilon$  and each dimension of the density ratio,  $Ld + 1$ , where the expectation is evaluated over the test samples. The mean square error is calculated by the average over 500 iterations.

Figure 2 shows the results. When the model is specified, i.e.,  $\delta = 0$  ( $\varepsilon = 0$ ), LMS estimator presents better performance than DRESS. Under the practical setup such as  $\delta > 1$ , however, we see that DRESS outperforms LMS estimator. The dependency on the dimension of the density-ratio model is not clearly detected in this experiment. Overall, larger density-ratio model presents rather unstable result. Indeed, in DRESS with large density ratio model, say the right bottom panel in Figure 2, the mean square error of DRESS can be large, i.e., the improvement is negative, even when the model misspecification  $\delta$  is large.

Next, we compare LMS estimator and DRESS with a nonparametric estimator of the density-ratio. Here, we use KuLSIF (Kanamori et al., 2012) as the density-ratio estimator. KuLSIF is a non-parametric estimator of the density-ratio based on the kernel method. The regularization is efficiently conducted to suppress the degree of freedom of the nonparametric model. In KuLSIF, the kernel function of the reproducing kernel Hilbert space corresponds to the basis function  $\phi(x)$ .

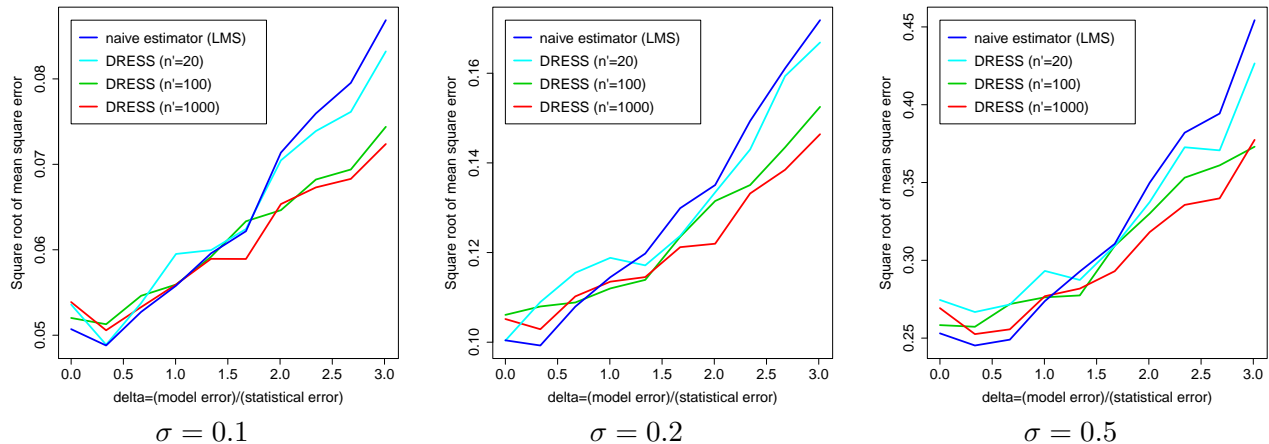


Figure 3: The square root of mean square errors of naive estimator and DRESS with  $n' = 20, 100, 1000$  are depicted as the function of  $\delta$ , where  $\delta$  is the normalized measure of the model misspecification. The sample size of the labeled data is  $n = 50$ , and  $\sigma$  is the standard deviation of the noise involved in the dependent variable  $y$ .

Under the setup of  $d = 10, n = 50, n' = 20, 100, 1000$  and  $\sigma = 0.1, 0.2, 0.5$ , we compute the mean square errors by the average over 100 iterations. In Figure 3, the square root of the mean square errors for LMS estimator and DRESS are plotted as the function of  $\delta$ , i.e.,  $(\text{model error})/(\text{statistical error})$ . When  $\delta$  is around 1, it is statistically hard to detect the model misspecification by the training data of the size  $n = 50$ . When the model is specified ( $\varepsilon = 0$ ), LMS estimator presents better performance than DRESS. Under the practical setup such as  $\delta > 1$ , however, we see that DRESS with KuLSIF outperforms LMS estimator. As shown in the asymptotic analysis, we notice that the sample size of the unlabeled data affects the estimation accuracy of DRESS. The numerical results show that DRESS with large  $n'$  attains the smaller error comparing to DRESS with small  $n'$ , especially when  $\delta > 1$  holds. In the numerical experiment, even DRESS with  $n = 50$  and  $n' = 20$  slightly outperforms LMS estimator. This is not supported by the asymptotic analysis. Hence, we need more involved theoretical study about the statistical feature of semi-supervised learning.

## 7.2 Classification problems

As a classification task, we use **spam** dataset in “kernlab” of R package (Karatzoglou et al., 2004). The dataset includes 4601 samples. The dimension of the covariate is 57, i.e.,  $\mathbf{x} = (x_1, \dots, x_{57})^T$  whose elements represent statistical features of each document. The output  $y$  is assigned to “spam” or “nonspam”.

For the binary classification problem, we use the logistic model,

$$P(\text{spam} | \mathbf{x}; \boldsymbol{\alpha}) = \frac{1}{1 + \exp\{-\alpha_0 - \sum_{d=1}^D \alpha_d x_d\}},$$

where  $D$  is the dimension of the covariate used in the logistic model. In numerical experiments,  $D$  varies from 10 to 57, hence, the dimension of the model parameter  $\boldsymbol{\alpha}$  varies from 11 to 58. We tested DRESS with KuLSIF (Kanamori et al., 2012) and MLE with  $n = 200, 500, 800$  randomly

chosen labeled training samples and  $n' = 100, 500, 1000, 2000$  unlabeled training samples. The remaining samples are served as the test data. The score function  $\mathbf{u}(x, y; \boldsymbol{\alpha}) = \nabla \log P(y|\mathbf{x}; \boldsymbol{\alpha})$  is used for the estimation.

Table 1 shows the prediction errors (%) with the standard deviation. We also show the p-value of the one-tailed paired  $t$ -test for prediction errors of DRESS and MLE. Small p-values denote the superiority of DRESS. We notice that p-value is small when the dimension  $D$  is not large. In other word, the numerical results meet the asymptotic theory in Section 6. For relatively high dimensional models, the prediction error of MLE is smaller than that of DRESS; see the row of  $D = 57$  in Table 1. The size of unlabeled data,  $n'$ , also affects the results. Indeed, the p-value becomes small for large  $n'$ . This result is supported by the asymptotic analysis presented in Section 6.

Table 1: Prediction errors (%) for DRESS with KuLSIF and MLE are shown. The p-values of the one-tailed paired  $t$ -test for prediction errors are also presented.

$n = 200, n' = 100$				$n = 500, n' = 100$				$n = 800, n' = 100$			
$D$	DRESS	MLE	p-value	DRESS	MLE	p-value		DRESS	MLE	p-value	
10	21.48±0.95	21.69±1.09	0.023	20.86±0.76	20.93±0.82	0.163		20.73±0.71	20.72±0.67	0.541	
20	18.81±1.30	18.54±1.42	0.987	17.15±0.79	17.16±0.90	0.424		16.63±0.68	16.93±0.87	0.000	
30	14.67±1.54	14.44±1.50	0.993	11.83±0.75	11.92±0.83	0.056		11.29±0.51	11.39±0.56	0.057	
40	16.16±1.79	16.06±1.83	0.910	12.18±0.81	12.19±0.84	0.410		11.24±0.60	11.40±0.62	0.005	
50	15.98±2.49	15.84±2.45	0.939	11.41±0.94	11.25±0.94	0.988		10.13±0.66	10.15±0.65	0.359	
57	15.08±2.64	15.01±2.67	0.777	10.83±1.06	10.59±0.90	1.000		9.07±0.61	8.98±0.70	0.959	
$n = 200, n' = 500$				$n = 500, n' = 500$				$n = 800, n' = 500$			
$D$	DRESS	MLE	p-value	DRESS	MLE	p-value		DRESS	MLE	p-value	
10	21.34±0.88	21.59±1.12	0.003	20.56±0.70	21.06±0.84	0.000		20.40±0.62	20.76±0.71	0.000	
20	18.58±1.40	18.60±1.45	0.406	16.76±0.79	17.10±0.96	0.000		16.51±0.67	16.95±0.90	0.000	
30	14.46±1.50	14.48±1.39	0.392	11.71±0.70	11.86±0.73	0.002		11.21±0.56	11.46±0.58	0.000	
40	15.88±1.98	15.83±2.05	0.759	11.96±0.79	12.04±0.77	0.035		11.13±0.56	11.41±0.62	0.000	
50	16.18±2.31	16.22±2.30	0.303	11.24±0.92	11.26±0.93	0.350		10.04±0.66	10.13±0.70	0.021	
57	14.88±2.82	14.77±2.77	0.933	10.83±1.07	10.61±0.98	1.000		8.79±0.70	8.81±0.63	0.319	
$n = 200, n' = 1000$				$n = 500, n' = 1000$				$n = 800, n' = 1000$			
$D$	DRESS	MLE	p-value	DRESS	MLE	p-value		DRESS	MLE	p-value	
10	21.26±0.96	21.74±1.28	0.000	20.57±0.74	21.02±0.80	0.000		20.29±0.61	20.74±0.64	0.000	
20	18.37±1.27	18.63±1.45	0.001	16.78±0.70	17.08±1.00	0.000		16.47±0.65	16.93±0.80	0.000	
30	14.53±1.51	14.60±1.42	0.089	11.73±0.67	12.04±0.78	0.000		11.16±0.62	11.43±0.69	0.000	
40	16.05±1.97	16.06±1.92	0.463	11.84±0.78	11.91±0.75	0.098		11.19±0.63	11.45±0.72	0.000	
50	15.58±2.16	15.52±2.10	0.703	11.20±0.86	11.20±0.86	0.566		9.94±0.75	10.06±0.80	0.006	
57	14.99±2.86	14.94±2.93	0.684	10.83±1.04	10.75±0.98	0.935		8.88±0.72	8.99±0.73	0.014	
$n = 200, n' = 2000$				$n = 500, n' = 2000$				$n = 800, n' = 2000$			
$D$	DRESS	MLE	p-value	DRESS	MLE	p-value		DRESS	MLE	p-value	
10	21.31±1.06	21.78±1.27	0.000	20.49±0.81	21.00±0.94	0.000		20.18±0.85	20.70±1.02	0.000	
20	18.36±1.35	18.62±1.51	0.008	16.79±0.86	17.18±1.09	0.000		16.37±0.80	16.88±0.97	0.000	
30	14.66±1.71	14.53±1.69	0.956	11.65±0.77	11.82±0.79	0.001		11.12±0.79	11.44±0.85	0.000	
40	15.78±1.76	15.60±1.74	0.985	11.81±0.90	12.10±0.97	0.000		10.94±0.81	11.33±0.79	0.000	
50	16.21±2.17	16.01±2.14	0.973	11.24±1.02	11.29±0.98	0.183		10.01±0.78	10.19±0.78	0.001	
57	14.87±2.57	14.95±2.55	0.170	10.52±1.13	10.56±1.14	0.187		8.71±0.79	8.91±0.84	0.000	

## 8 Conclusion

In this paper, we investigated the semi-supervised learning with density-ratio estimator. We proved that the unlabeled data is useful when the model of the conditional probability  $p(y|x)$  is misspecified. This result agrees to the result given by Sokolovska, et al. (Sokolovska et al., 2008), in which the weight function is estimated by using the estimator of the marginal probability  $p(x)$  under a specified model of  $p(x)$ . The estimator proposed in this paper is useful in practice, since our method does not require the well-specified model for the marginal probability. Numerical experiments present the effectiveness of our method. We are currently investigating semi-supervised learning from the perspective of semiparametric inference with missing data. A positive use of the statistical paradox in semiparametric inference is an interesting future work for semi-supervised learning.

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